

# CLASSICAL MARKOVIAN KINETIC EQUATIONS: EXPLICIT FORM AND H-THEOREM

Constantinos Tzanakis

University of Crete, 74100 Rethymnon, Crete, Greece

Alkis P. Grecos<sup>†</sup>

Service de Physique Statistique et plasmas

Université Libre de Bruxelles, Campus Plaine (CP.231)

1050 Bruxelles, Belgium

## ABSTRACT

The probabilistic description of finite classical systems often leads to linear kinetic equations. A set of physically motivated mathematical requirements is accordingly formulated. We show that it necessarily implies that solutions of such a kinetic equation in the Heisenberg representation, define Markov semigroups on the space of observables. Moreover, a general  $H$ -theorem for the adjoint of such semigroups is formulated and proved provided that at least locally, an invariant measure exists. Under a certain continuity assumption, the Markov semigroup property is sufficient for a linear kinetic equation to be a second order differential equation with nonnegative-definite leading coefficient. Conversely it is shown that such equations define Markov semigroups satisfying an  $H$ -theorem, provided there exists a nonnegative equilibrium solution for their formal adjoint, vanishing at infinity.

## 1. INTRODUCTION

In a probabilistic description of classical systems with a finite number of degrees of freedom, one often encounters *linear, autonomous, evolution equations* of the form

$$\frac{\partial f}{\partial t} = Z_S f. \quad (1.1)$$

Such equations, which henceforth, and for the sake of brevity, will be called kinetic equations, are assumed to determine the time evolution of the statistical state of the system. In this context, *states are taken to be probability densities on the phase space*,

---

<sup>†</sup>Association Euratom-Etat Belge

the manifold of the dynamical variables characterizing the system, while observables  $A$  are simply (sufficiently well-behaved, real) phase-space functions. Furthermore, expectation values are obtained via some bilinear form  $w$  on the cartesian product of the spaces of states and observables

$$\langle A \rangle_f \equiv w(f, A), \quad (1.2)$$

provided they remain finite for all observables, i.e.  $|w| < +\infty$ . If the evolution of observables is considered, an equation of the form

$$\frac{\partial A}{\partial t} = Z_O A, \quad (1.1')$$

should hold, with  $Z_O$  a formal adjoint in the sense that

$$w(f, Z_O A) = w(Z_S f, A) \quad (1.3)$$

Here it is being assumed that  $w$  separates the states and observables (equivalently:  $w$  is nondegenerate) and

$$w(f_t, A) = w(f, A_t)$$

i.e. the two pictures are essentially equivalent. Typical examples are well known kinetic equations, like those of Kramers, Fokker-Planck or the (linear) Boltzmann and Landau equations<sup>1-3</sup>. Such equations result by applying some more or less systematic approximation scheme based on a perturbation analysis of the exact microscopic dynamics of the system under consideration<sup>3,4</sup>, or by applying stochastic methods<sup>2,5</sup>, based on assumptions concerning the behaviour of a large number of microscopic events characterizing the system. For classical open systems weakly interacting with large equilibrium baths, kinetic equations have been derived<sup>6,7</sup> using techniques similar to those developed for quantum systems<sup>8</sup>. On the other hand, some ‘markovianization’ procedures imposed on the exact dynamics may lead to inconsistent equations<sup>9</sup>. Note that in such derivations, expansions with respect to some appropriate parameter are used, implying that  $Z_S$  or  $Z_O$  are differential operators of some order, depending on the approximation.

However in the physics literature, not sufficient attention has been given to a general presentation of the structure and properties of such *classical* (“Markovian”) kinetic equations, *independently of the method used to derive them*<sup>10</sup>. In our opinion this seems necessary at least for two reasons :

(a) as already mentioned, proposed perturbation schemes may lead to results incompatible with a probabilistic interpretation, particularly, violation of positivity of the states<sup>9</sup>

(b) derivations based on the theory of stochastic processes *a priori* impose conditions on the physical characteristics of the systems studied (e.g. postulate a master evolution equation for the states, like the Chapman-Kolmogorov equation, on which approximations are subsequently made).

Instead, our aim in this paper is to provide a mathematically rigorous and physically adequate framework for the study of such kinetic equations, and examine certain of the properties of their solutions, formally determined by one parameter semigroups  $V_t = e^{Zst}$ . Specifically, we give *minimal* conditions under which

- (1) Eq. (1.1) *does* indeed define rigorously a semigroup of solutions capable of a probabilistic interpretation, particularly preserving positivity,
- (2) it is possible to characterize  $Z_S$  and  $Z_O$  and explicit their general form if they are differential operators,
- (3) an H-theorem for arbitrary continuous convex functionals of the state can be proved.

In this way, the outline of the formal framework for a probabilistic description of finite classical systems given at the beginning of this section, is made precise and kinetic equations like (1.1), (1.1') become in principle mathematically and physically meaningful. Our approach is similar to that followed in defining dynamical semigroups for quantum systems<sup>11</sup>. To this end, we notice that (1.2) is essentially a duality relation, suggesting that states are linear functionals defined on observables. Then the interpretation of states as probability densities in (1.1) implies that observables are *bounded* functions in phase-space. Then, in view of (1.2), finite expectation values for *all* observables naturally leads to an extension of the state-space beyond probability densities, so that all linear functionals defined on bounded functions are included. In section 2, these qualitative remarks are precisely formulated, thus establishing a sufficiently wide mathematical framework for the derivation of rigorous results. In particular it will be seen that *kinetic equations like (1.1') should necessarily define a Markov semigroup of solutions on the (Banach) space of observables*. In section 3 we collect basic theorems concerning the generator of a Markov semigroup. Some proofs are presented, mainly

because they are partly used as intermediate steps toward other results so that the paper is sufficiently self-contained. In section 4 we show rigorously that the only differential operators that are candidates as generators of Markov semigroups, are at most of the 2nd order, namely (degenerate in general) elliptic operators (Lemma 4.1). We further supply a complete proof of the fact that under a certain continuity assumption, well-known in the theory of stochastic processes, eq(4.1), the generator of a Markov semigroup is indeed a differential operator (theorem (4.1)). The *converse problem* is considered in section 5, where we show that under mild regularity conditions, in general *degenerate* elliptic operators generate Markov semigroups *globally* defined on the space of observables. This generalizes classical results on local solutions of nondegenerate elliptic equations. Finally in section 6, *a general H-theorem for arbitrary continuous functionals on the state-space is formulated and proved for any* (and not only for a diffusion type) *Markov semigroup, under the assumption that an invariant measure exists, which for a diffusion-type semigroup is implied by the existence of an equilibrium solution  $\rho_0$  of (1.1)* (theorem 6.1). It should be emphasized at this point that  $\rho_0$  *need not be a probability density*, i.e. integrable on the whole phase-space of the system (e.g. for particle systems, in position as well as in velocity space). This is a *global* formulation of the H-theorem (corollary (6.1)) to be contrasted to the *local* one given as an entropy continuity equation, and usually obtained in cases the kinetic equation for the states has a nonintegrable stationary solution. Moreover, it will become apparent that *the existence of such a solution* (satisfied by the formalism of Refs.6, 7) implies that the Markov semigroup property (specifically, positivity conservation) is (essentially) *equivalent to the existence of H-functions*.

## 2. MATHEMATICAL ASSUMPTIONS AND THEIR PHYSICAL MOTIVATION: MARKOV SEMIGROUPS

As already mentioned, inherent to kinetic equations like (1.1) is a probabilistic interpretation. Motivated by the preceding qualitative discussion, we introduce a *minimal* set of assumptions to fix an appropriate mathematical framework for states and observables of a finite classical system and for their time evolution given by kinetic equations like (1.1), (1.1'). Though the interpretation of states is better suited to supply the *physical* motivation for such assumptions, it is *mathematically* more convenient to work with observables. This is suggested by theorem 2.1 below and will become more evident in

sections 3-5. The results thus obtained will enable us to return to the state space when formulating and proving the H-theorem in the last section.

We consider admissible observable quantities  $A$  as (real) bounded continuous functions on the phase space  $X$ , that remain finite at infinity,  $X$  being a differentiable manifold (e.g. the phase-space of a Hamiltonian system). It is convenient to embed them in a complex linear space (and extend  $w$  in (1.2) to a sesquilinear form). Thus we introduce

**Assumption ( $A_1$ )** : The phase-space  $X$  of a system is a differentiable manifold, and observables belong to  $C(X_\infty, \mathbb{C})$ , the space of all continuous complex valued functions having a finite limit at infinity.

Here,  $X_\infty$  is  $X$  together with the infinite point (more precisely, the one-point compactification of  $X$ ). Then continuous functions  $A$ , having a finite limit at infinity (in particular constant functions)<sup>12</sup> can be identified with continuous functions on  $X_\infty$ , by defining  $A(\infty)$  to be this finite limit. Thus observables belong to  $C(X_\infty, \mathbb{C})$  which is a Banach space with norm  $\|A\| = \sup_{x \in X_\infty} |A(x)|$ .

In section 1, it has been suggested that states  $l$  are linear functionals on the space of observables, their values  $l(A)$  giving expectations. Then, their probabilistic interpretation requires them to be positive, i.e.  $l(A) \geq 0$  for  $A \geq 0$ , since expectation values of nonnegative random variables are nonnegative (notice that  $l$  is real in this case). Then  $l$  is bounded with bound  $\|l\| = l(1)$ <sup>13</sup>, hence  $l$  is continuous on  $C(X_\infty, \mathbb{C})$  that is  $l \in C^*(X_\infty, \mathbb{C})$  where  $S^*$  is the Banach dual of a normed space  $S$ . The above comments are summarized in

**Assumption ( $A_2$ )** : If  $C(X_\infty, \mathbb{C})$  contains the observables  $A$ , then states  $l$  are positive linear functionals on it and expectation values are given by  $l(A)$ .

We remark here, that states thus introduced, extend the class of states defined by probability densities, this extended class being characterized as probability measures by the Riesz-Markov theorem below<sup>13,14</sup>.

**Theorem 2.1** (i) For every positive  $\ell \in C^*(X_\infty, \mathbb{C})$  there exists a unique *positive* (regular) Borel measure  $\mu$  such that

$$\ell(A) = \int A(x) d\mu(x) , \quad \|\ell\| = \ell(1) = \mu(X_\infty) \quad (2.1)$$

(ii) More generally, if  $\ell \in C^*(X_\infty, \mathbb{C})$ , there exists a unique *complex* Borel measure  $\mu$  such that (2.1) holds and  $\|\ell\| = |\mu|(X_\infty)$ , where  $|\mu|$  is the total variation of  $\mu$ <sup>14</sup>.

*Remarks:* In the present work all measures are *regular Borel measures*. The theorem is valid if  $C(X_\infty, \mathbb{C})$  is replaced by  $C_0(X, \mathbb{C})$  or  $C_c(X, \mathbb{C})$ , the spaces of functions vanishing at infinity or having compact support respectively. Finally, we notice that unbounded phase space functions such as polynomials, have been excluded from observables, since for such functions it is impossible to have finite expectation values for *all* states.

Having established states and observables as elements of dual Banach spaces, we introduce for their time evolution (1.1), (1.1')

**Assumption** ( $A_3$ ): Equation (1.1') has a well-posed initial-value problem, that is: for given initial data, the solution is unique for  $t > 0$ , it depends continuously on the initial data (small changes in the initial data imply small changes in the solution, in the sense of the Banach space norm) and expectations are continuous in  $t$ .

Notice that  $A_3$ , proposition 2.2 below and  $A_2$  imply that  $A_3$  holds for (1.1) as well and by the linearity of (1.1') nonuniqueness for one initial condition implies nonuniqueness for all. It is well known that  $A_3$  implies

**Proposition 2.1** If (1.1') is linear, autonomous and has a well-posed initial value problem on some set  $U$  of the Banach space of observables, then its solutions  $A(t)$  with initial conditions  $A$ , uniquely define a s-continuous one-parameter semigroup of operators  $T_t A \equiv A(t)$  on the Banach subspace  $B \equiv \bar{U}$  (from now on the prefix s or w means strong or weak respectively and  $\bar{U}$  is the s-closure of  $U$ ).

Here we used that continuity of expectation values imply w-continuity of  $T_t$  for  $t = 0$ , which is equivalent to its s-continuity for  $t \geq 0$ <sup>15</sup> and

**Definition 2.1** A (one-parameter s-continuous) semigroup (of operators) on a Banach space  $B$ , is a family of bounded linear operators  $\{T_t, t \geq 0\}$ , such that:

- (i)  $T_{t+s} = T_t T_s$ , (ii)  $s\text{-}\lim_{t \rightarrow t_0} T_t A = T_{t_0} A \quad \forall A \in B$ ,

Its generator  $Z$  is defined by

$$\mathcal{D}(Z) = \left\{ A \in B : s\text{-}\lim_{t \rightarrow 0^+} \frac{T_t A - A}{t} \text{ exists} \right\}, \quad Z A = s\text{-}\lim_{t \rightarrow 0^+} \frac{T_t A - A}{t} \quad (2.2)$$

It is well-known that the *converse* holds<sup>16,17</sup> - derivatives and integrals being defined using the Banach space norm<sup>16</sup>.

**Theorem 2.2** Let  $T_t$  be a semigroup on a Banach space, s-continuous at  $t = 0$  on a Banach subspace  $B$ . Define  $Z$  by (2.2) ( $\mathcal{D}(Z) \neq \emptyset$ ). Then

- (a) on  $B$ ,  $T_t$  is uniquely defined by  $Z$  and is s-continuous for  $t \geq 0$ ;  $B$  is  $T_t$ -invariant,

norm-closed and

$$T_0|_B = I, \quad B = \overline{\mathcal{D}(Z)}, \quad \|T_t\| \leq Me^{at} \quad \text{for some } M \geq 1, \quad a \in \mathbb{R} \quad (2.3)$$

(b)  $Z$  is a closed operator, for  $A \in \mathcal{D}(Z)$ ,  $T_t A$  is  $s$ -differentiable (cf.(2.2)), hence  $T_t(\mathcal{D}(Z)) \subseteq \mathcal{D}(Z)$

$$\frac{\partial T_t A}{\partial t} = Z T_t A = T_t Z A \quad T_t A - A = \int_0^t T_s A ds \quad (2.4)$$

and  $T_t A$  is the unique solution of (2.4) (cf.(1.1')) on  $B$  with initial condition  $A$ , satisfying  $\|A_t\| \leq ce^{kt}$  for  $c, k$  constants.

(c) For  $\lambda > a$  (cf.(2.3))  $\lambda - Z : \mathcal{D}(Z) \rightarrow B$  is invertible, its inverse  $R_\lambda$ , the resolvent of  $Z$ , is bounded and

$$R_\lambda A = \int_0^\infty e^{-\lambda t} T_t A dt, \quad \|R_\lambda\| \leq \frac{M}{\lambda - a} \quad (2.5)$$

The adjoint semigroup  $T_t^*$  is everywhere defined on  $B^*$  by  $(T_t^* \ell)(A) = \ell(T_t A)$ . Similarly since  $Z$  is densely defined on  $B$ , its adjoint  $Z^*$  is defined for all  $\ell \in B^*$  for which  $A \rightarrow \ell(ZA)$  is bounded, as the unique bounded extension of this functional to  $B$ . Thus  $(Z^* \ell)(A) = \ell(ZA) \forall A \in \mathcal{D}(Z)$ . Now, unless  $B$  is a reflexive Banach space neither  $T_t^*$  is  $s$ -continuous on  $B^*$  nor  $Z^*$  is its generator. Therefore (1.1'), (1.1) are not simply adjoint equations. However we have <sup>17</sup>

**Proposition 2.2** Let  $T_t$  be a  $s$ -continuous semigroup on the Banach space  $B$ , with generator  $Z$ . Then its adjoint  $T_t^*$  is  $s$ -continuous on a (presumably proper) Banach subspace of  $B^*$ , uniquely determined on  $B^*$  by its generator however, and for which  $Z^*$  is an extension.

Thus going back to (1.1), (1.1'), either  $Z_S$  or  $Z_O^*$  can be taken as the generator in the evolution equation for the states without any inconsistency. In connection with  $A_2$  we require conservation of positivity and of normalization of the states for all times, that are indispensable for their probabilistic interpretation

**Assumption ( $A_4$ ):** (a) For  $t > 0$ ,  $\ell$  positive implies  $T_t^* \ell$  positive; (b)  $T_t^* \ell(1) = \ell(1)$  for any state  $\ell$ .

By  $A_4$  and theorem 2.1

$$T_t A \geq 0 \quad \text{for continuous } A \geq 0 \quad \text{in } B, \quad T_t 1 = 1 \quad (2.6)$$

which imply<sup>17</sup> that  $\|T_t\| = \|T_t(1)\| = 1$ , i.e.  $T_t$  (hence  $T_t^*$ ) is a *contraction semigroup* ( $\|T_t\| \leq 1$ ).

In summary, assumptions  $A_1$ - $A_4$ , sufficiently well justified upon physical and mathematical considerations, imply that linear autonomous kinetic equations conserving the probabilistic interpretation of states, *necessarily generate Markov semigroups on  $C(X_\infty, \mathbb{C})$ , the space of observables, i.e. a positivity and normalization preserving  $s$ -continuous semigroup* (cf.(2.6)). In the next two sections their properties are considered (proof of their 1-1 correspondence with time-homogeneous Markov processes is outlined in Appendix 1).

### 3. GENERAL RESULTS ON THE GENERATOR OF A MARKOV SEMIGROUP

Here we summarize results on the generator of a Markov semigroup. Though we follow mainly Ref.17, some proofs are slightly modified so that a coherent presentation results. The Hille-Yosida theorem is in our case<sup>15,17</sup>

**Proposition 3.1** A closed, densely defined operator  $Z$  on a (presumably complex) Banach space  $B$  is the generator of a  $s$ -continuous contraction semigroup of operators iff its resolvent  $R_\lambda = (\lambda - Z)^{-1}$  is an everywhere defined bounded operator for  $\lambda > 0$  and

$$\|R_\lambda\| \leq 1/\lambda, \quad \lambda > 0 \quad (3.1)$$

*Remark:* The resolvent set of  $Z$ , i.e. those  $z \in \mathbb{C}$  such that  $R_z$  is everywhere defined, contains  $\mathbb{R}^+$ , and since  $Z$  is closed, it is an open set, in particular  $\mu$  belongs there for  $|\mu - \lambda| \leq \frac{1}{\|R_\lambda\|}$ .  $R_\lambda$  is a closed (hence bounded, by the closed-graph theorem) operator on  $B$ .

Contractivity of a semigroup is related to the dissipativity of its generator: by the Hahn-Banach theorem, in a normed space  $B$  and for every  $A \in B$  there exists an (in general nonunique)  $\ell \in B^*$  such that<sup>15</sup>

$$\|\ell\| = 1 \quad , \quad \ell(A) = \|A\| \quad \text{equivalently} \quad \|\ell\| = \|A\| \quad \ell(A) = \|A\|^2 \quad (3.2)$$

Thus we give:



**Definition 3.1** An operator  $Z$  on a normed space  $B$  is dissipative if and only if for every  $(\ell, A) \in B^* \times B$  satisfying (3.2) ( $\text{Re}$  denoting the real part)

$$\text{Re } \ell(ZA) \leq 0 \quad (3.3)$$

*Remark:* For a Hilbert space with scalar product  $\langle, \rangle$ , (3.3) is equivalent to  $\text{Re } \langle A, ZA \rangle \leq 0$ , hence  $\|T_t A\|^2$  decreases monotonically in time (cf.(2.4)). This is closely related to an  $H$ -theorem for the adjoint equation (section 6).

**Proposition 3.2** If  $Z$  is a densely defined *closed* operator on a Banach space  $B$ , the following are equivalent:

- (a)  $Z$  generates a  $s$ -continuous contraction semigroup on  $B$ .
- (b) (i)  $\text{Range}(\lambda - Z) = B \quad \forall \lambda > 0$ , (ii)  $Z$  is dissipative
- (c) (i)  $\exists \lambda > 0 : \text{Range}(\lambda - Z) = B$ , (ii)  $\forall A \in B \exists \ell \in B^*$  so that (3.2), (3.3) hold.

**Proof:** (a) $\Rightarrow$ (b): Condition (b,i) is part of proposition 3.1 Take  $\ell, A$  as in (3.2). Then by the continuity of  $\ell$  and (3.2)

$$\text{Re } \ell(ZA) = \text{Re } \lim_{t \rightarrow 0^+} \frac{\ell(T_t A) - \|A\|}{t} \leq \text{Re } \lim_{t \rightarrow 0^+} \frac{(\|T_t\| - 1)\|A\|}{t} \leq 0$$

(b) $\Rightarrow$ (c) trivial

(c) $\Rightarrow$ (a) for  $A \in \mathcal{D}(Z)$  take  $\ell$  as in (3.2). Then for *any*  $\mu > 0$

$$\|(\mu - Z)(A)\| \geq |\ell((\mu - Z)A)| = |\mu\|A\| - \ell(ZA)| \geq \mu\|A\|$$

hence  $\mu - Z$  is 1-1 in its range, and if this is equal to  $B$ , then  $\mu$  is in the resolvent set of  $Z$  and  $\|R_\mu\| \leq \frac{1}{\mu}$ ; in particular  $\frac{1}{\|R_\lambda\|} \geq \lambda$ . By the remark in proposition 3.1, every  $\mu \in (0, \frac{3\lambda}{2}] \subseteq (0, \lambda + \frac{1}{\|R_\lambda\|})$  is in the resolvent set of  $Z$ . By induction all  $\mu \in (0, (\frac{3}{2})^n \lambda]$  are in the resolvent set, for all  $n \in \mathbb{N}$ . Q.E.D.

Modifying slightly the proof (c) $\Rightarrow$ (a) above we obtain <sup>17</sup>

**Corollary 3.1** If  $Z$  is a densely defined *closable* operator on the Banach space  $B$  with  $\text{Range}(\lambda - Z)$  dense in  $B$  for *some*  $\lambda > 0$  and condition (c,ii) of proposition 3.2 holds, then its closure  $\tilde{Z}$  generates a  $s$ -continuous semigroup on  $B$ .

*Remark:* From (2.10-11) conservation of *positivity and normalization* on  $C(X_\infty, \mathbb{C})$ , *imply dissipativity*. For a *partial* converse we have

**Proposition 3.3** A  $s$ -continuous contraction semigroup  $T_t$  of operators on  $C(X_\infty, \mathbb{C})$  with generator  $Z$ , is positivity-preserving if  $(ZA)^* = ZA^*$ , and

$$\text{if } A(x_0) \geq A(x) \quad \forall x \in X_\infty \quad \text{then} \quad ZA(x_0) \leq 0 \quad (3.4)$$

**Proof:** By proposition 3.1, every  $\lambda > 0$  is in the resolvent set of  $Z$  and since  $\mathcal{D}(R_\lambda) = C(X_\infty, \mathbb{C})$ , we shall show that  $(\lambda - Z)A \geq 0 \Rightarrow A \geq 0$ . Suppose  $A$  takes negative values on  $X_\infty$ , with an absolute minimum  $A(x_0)$ . By (3.4)  $(\lambda - Z)A(x_0) < 0$  for any  $\lambda > 0$  and by proposition 3.1, for any  $\lambda > 0$   $\|\lambda(\lambda R_\lambda - I)\| \leq 2\lambda \forall \lambda > 0$ . Therefore  $T_t^\lambda \equiv e^{-\lambda t} e^{\lambda^2 R_\lambda t}$  is a well-defined, positivity-preserving  $s$ -continuous semigroup and  $\lambda(\lambda R_\lambda - I) = \lambda Z R_\lambda$ . From this follows that  $s\text{-}\lim_{\lambda \rightarrow +\infty} \lambda(\lambda R_\lambda - I)A = ZA$  for  $A \in \mathcal{D}(Z)$ , which implies  $s\text{-}\lim_{\lambda \rightarrow +\infty} T_t^\lambda = T_t A$  uniformly in  $t$  on bounded intervals<sup>17</sup>. Hence  $T_t A \geq 0$  for  $A \geq 0$  Q.E.D.

*Remark:* If  $1 \in \mathcal{D}(Z)$ , (3.4) implies  $Z(1) = 0$ , hence  $T_t 1 = 1$ .

Proposition 3.2 and theorem A.1.1 give the characterization of the generator of a Markov semigroup by (see Ref.34, section 7.7 for a slightly different formulation)

**Theorem 3.1** Let  $Z$  be a densely defined closed operator on  $C(X_\infty, \mathbb{C})$ . Then the following are equivalent:

- (a)  $Z$  generates a Markov semigroup  $T_t$
- (b) (i)  $1 \in \mathcal{D}(Z)$ ,  
(ii)  $\exists \lambda > 0 : \text{Range}(\lambda - Z) = C(X_\infty, \mathbb{C})$ ,  
(iii)  $(ZA)^* = ZA^* \forall A \in \mathcal{D}(Z)$ ,  
(iv) (3.4) holds.

**Proof:** (a)  $\Rightarrow$  (b). (i) follows from (2.6), (ii) from proposition 3.1 since  $T_t$  is a contraction semigroup. By theorem A.1.1 and (A.1.2) both (iii), (iv) are evident.

(b)  $\Rightarrow$  (a). Let  $A \in \mathcal{D}(Z)$ . Since  $X_\infty$  is compact,  $|A|$  continuous,  $\|A\| = |A(x_0)|$  for some  $x_0 \in X_\infty$ . Without loss of generality let  $A(x_0) > 0$  and  $\delta_{x_0}$  be the  $\delta$ -function at  $x_0$ , which is a positive linear functional on  $C(X_\infty, \mathbb{C})$ , hence  $\|\delta_{x_0}\| = \delta_{x_0}(1) = 1$ . Then  $\|A\| = A(x_0) = \delta_{x_0}(A) \geq A(x) \forall x \in X_\infty$ , so that by (3.4)  $\delta_{x_0}(ZA) = ZA(x_0) \leq 0$ . Hence by (ii) and proposition 3.2,  $Z$  generates a contraction semigroup, which by (ii), (iii) and proposition 3.3 is positivity-preserving. Since  $\mathcal{D}(Z) \ni 1$ ,  $T_t 1 = 1$  by the remark to proposition 3.3. Q.E.D.

*Remark:* Proposition 3.3 and theorem 3.1 show that (3.4) is the crucial condition relating dissipativity with conservation of positivity (see end of section 4 and section 6).

#### 4. DIFFERENTIAL OPERATORS GENERATING MARKOV SEMIGROUPS

In view of the last remark we explicit the form of the generator of a Markov semigroup that is a *differential* operator, since kinetic equations are often given by such operators. We first prove<sup>18,19</sup>

**Lemma 4.1** Let  $Z$  be a differential operator of order  $k$ , defined on  $C^k(\mathbb{R}^n, \mathbb{R})$  and suppose that for any  $f \in \mathcal{D}(Z)$ , if  $f(\vec{x}_0) \geq f(\vec{x}) \forall \vec{x} \in \mathbb{R}^n$  then  $Zf(\vec{x}_0) \leq 0$ . Then  $Z$  is at most a 2nd order differential operator with nonnegative-definite 2nd order coefficient.

**Proof:** (i) Let  $n = 1$ . By the remark to proposition 3.3,  $Z$  has no zeroth order term. Suppose  $Z$  has the form

$$Z = c_1(x) \frac{d}{dx} + c_2(x) \frac{d^2}{dx^2} + c_k(x) \frac{d^k}{dx^k} \quad k \geq 3$$

and that  $c_k(x_0) \neq 0$  for some  $x_0 \in \mathbb{R}$ . Let

$$g(x) = -\epsilon(x - x_0)^2 + a(x - x_0)^k, \quad \epsilon > 0, a \in \mathbb{R}$$

Clearly  $g$  has a local maximum zero at  $x_0$ . There is a neighborhood  $N(x_0)$  with compact closure, in which  $g(x) \leq g(x_0) = 0$ . Let  $\tilde{f}(x)$  be a  $C^k$ -function with compact support,  $\tilde{f}(x) \leq 0$  on  $\mathbb{R} - N(x_0)$  having the same partial derivatives with  $g$  up to order  $k$ , on the boundary of  $N(x_0)$ . Then

$$f(x) = \begin{cases} g(x) & , x \in N(x_0) \\ \tilde{f}(x) & , x \in \mathbb{R} - N(x_0) \end{cases}$$

is a  $C^k$ -function with  $f(x) \leq f(x_0) = 0 \forall x \in \mathbb{R}$  and  $Zf(x_0) = -2\epsilon c_2(x_0) + k!ac_k(x_0)$ . Since  $k > 2$ , appropriate choice of  $a$ , makes it positive, unless  $c_k(x_0) = 0$ .

By a similar argument  $c_2(x) \geq 0 \forall x \in \mathbb{R}$  (for any  $x_0 \in \mathbb{R}$  take  $g(x) = -\epsilon(x - x_0)^2, \epsilon > 0$ ).

(ii) For  $n > 1$  let  $Z$  contain a term of the form  $c(\vec{x})\partial_{i_1}^{a_1}\partial_{i_2}^{a_2}\dots\partial_{i_\ell}^{a_\ell}$ , where  $a_1 + a_2 + \dots + a_\ell = k > 2$  and  $\partial_i = \frac{\partial}{\partial x^i}$ . The proof can be repeated, starting with a  $\vec{x}_0$  for which  $c(\vec{x}_0) \neq 0$  and

$$g(\vec{x}) = a(x^{i_1} - x_0^{i_1})^{a_1} \dots (x^{i_\ell} - x_0^{i_\ell})^{a_\ell} - \epsilon \sum_{i=1}^n (x^i - x_0^i)^2$$

since it has a local maximum at  $\vec{x}_0$ . With  $g(\vec{x}) = -\sum_{i,j=1}^n \lambda_i \lambda_j (x^i - x_0^i)(x^j - x_0^j)$ ,  $\lambda_i \in \mathbb{R}$ , proceeding as before we obtain  $Zf(\vec{x}_0) = -\sum_{i,j=1}^n a_{ij}(\vec{x}_0) \lambda_i \lambda_j \leq 0$  where  $a_{ij}$  is the 2nd order coefficient of  $Z$ . Q.E.D.

**Remark:** The proof above is local. Therefore working in some local coordinates of a differentiable manifold and using its local compactness, so that  $N(\vec{x}_0)$ , hence  $\tilde{f}$  above exist, the same proof holds.

Now  $C_c^2(\mathbb{R}^n) \subseteq C(\mathbb{R}_\infty^n)$ , with the identification of continuous functions of  $\mathbb{R}^n$  having a finite limit at  $\infty$  with elements of  $C(\mathbb{R}_\infty^n)$  made in section 2. Then the following theorem supplies a *sufficient* condition for the generator of a markov semigroup to be a differential operator<sup>20</sup>.

**Theorem 4.1** Let  $T_t$  be a Markov semigroup on  $C(\mathbb{R}_\infty^n, \mathbb{C})$  with generator  $Z$  and suppose that

- (i)  $C_c^2(\mathbb{R}^n) \subseteq \mathcal{D}(Z)$
- (ii) The transition probability measure  $p(t, \vec{x}, \cdot)$  of the corresponding Markov process (see appendix 1) satisfies

$$\lim_{t \rightarrow 0^+} \frac{p(t, \vec{x}, N)}{t} = \chi_N(\vec{x}) \quad \text{uniformly in } \vec{x} \quad (4.1)$$

Then

$$Zf(\vec{x}) = b_i(\vec{x})\partial_i f(\vec{x}) + a_{ij}(\vec{x})\partial_i \partial_j f(\vec{x}) \quad f \in C^2(\mathbb{R}^n) \quad (4.2)$$

$b_i, a_{ij}$  are continuous, real-valued functions,  $a_{ij}$  is a nonnegative-definite matrix  $\forall \vec{x} \in \mathbb{R}^n$ ,  $\chi_N$  is the characteristic function of  $N$  and the summation convention is henceforth assumed.

**Proof:** Let  $\vec{x}_0 \in \mathbb{R}^n$ , and for  $f \in C_c^2(\mathbb{R}^n)$  consider its 2nd order Taylor polynomial at  $\vec{x}_0$ , denoting by  $\tilde{f}(\vec{x})$  the corresponding remainder. By Taylor's theorem, for every  $\epsilon > 0$ ,  $\tilde{f}(\vec{x}) \leq \epsilon \|\vec{x} - \vec{x}_0\|^2$  in some neighborhood  $N(\vec{x}_0)$ . Put

$$g_\epsilon(\vec{x}) = \begin{cases} \epsilon \|\vec{x} - \vec{x}_0\|^2 & , \vec{x} \in N(\vec{x}_0) \\ \sigma(\vec{x}) & , \vec{x} \in \mathbb{R}_\infty^n - N(\vec{x}_0) \end{cases}$$

where  $\sigma(\vec{x}) \in C_c^2(\mathbb{R}^n)$  is nonnegative and it and its first two partial derivatives coincide with those of  $\tilde{f}$  on  $\partial N(\vec{x}_0)$  (without loss of generality we take  $\overline{N(\vec{x}_0)}$  compact). Then  $|\tilde{f}(\vec{x})| \leq \epsilon g_\epsilon(\vec{x})$ ,  $\vec{x} \in N(\vec{x}_0)$  and

$$|Z\tilde{f}(\vec{x}_0)| = \lim_{t \rightarrow 0^+} \left| \frac{1}{t} \int_{\mathbb{R}_\infty^n - N(\vec{x}_0)} \tilde{f}(\vec{y}) p(t, \vec{x}_0, d\vec{y}) + \frac{1}{t} \int_{N(\vec{x}_0)} \tilde{f}(\vec{y}) p(t, \vec{x}_0, d\vec{y}) \right|$$

By (4.1)  $|\frac{1}{t} \int_{\mathbb{R}_\infty^n - N(\vec{x}_0)} \tilde{f}(\vec{y}) p(t, \vec{x}_0, d\vec{y})| \leq \|\tilde{f}\| o(1)$ . On the other hand, since  $g_\epsilon \geq 0$   $\frac{1}{t} \int_{N(\vec{x}_0)} \tilde{f}(\vec{y}) p(t, \vec{x}_0, d\vec{y}) \leq \frac{\epsilon}{t} \int g_\epsilon(\vec{y}) p(t, \vec{x}_0, d\vec{y})$ . Therefore  $|Z\tilde{f}(\vec{x}_0)| \leq \epsilon Zg_\epsilon(\vec{x}_0)$ . But  $\epsilon$  is arbitrary, hence  $Z\tilde{f}(\vec{x}_0) = 0$ .

Considering the functions  $f^i(\vec{x}) = x^i - x_0^i$ ,  $f^{ij}(\vec{x}) \equiv (x^i - x_0^i)(x^j - x_0^j)$  in  $N(\vec{x}_0)$ , extended to  $C_c^2(\mathbb{R}^n)$ -functions and using (4.1) we get

$$Zf^i(\vec{x}) = \lim_{t \rightarrow 0^+} \frac{1}{t} \int_{N(\vec{x}_0)} p(t, \vec{x}, d\vec{y})(y^i - x^i)$$

$$Zf^{ij} = \lim_{t \rightarrow 0^+} \frac{1}{t} \int_{N(\vec{x}_0)} p(t, \vec{x}, d\vec{y})(y^i - x^i)(y^j - x^j)$$

Returning to  $f$  and using this and that  $Z(1) = 0$ , we obtain  $Z\tilde{f}(\vec{x}_0) = 0$ . Since  $\vec{x}_0$  is arbitrary, (4.2) follows with  $b_i(\vec{x}) = Zf^i(\vec{x})$ ,  $a_{ij} = \frac{1}{2}Zf^{ij}(\vec{x})$ . By the definition of  $Z$ ,  $b_i, a_{ij}$  are continuous and evidently  $a_{ij}(\vec{x})$  is nonnegative-definite. Q.E.D.

*Remarks:*

- (a) Eq(4.1) implies the existence of the first two moments of  $p(t, \vec{x}, \cdot)$  and Lemma 4.1 that all higher moments vanish<sup>21</sup>. Notice that in the theory of stochastic processes, (4.2) is usually derived by assuming (4.1) *and the existence* of the first two moments of  $p$ , from which the vanishing of higher moments follows<sup>5</sup>. Notice also that (4.1) implies uniform stochastic continuity of  $p(t, \vec{x}, N)$ , (A.1.3).
- (b) For arbitrary differentiable manifolds, theorem 4.2 holds, since only local compactness of  $\mathbb{R}^n$  and Taylor's theorem are used.
- (c) The theorem is true if  $\mathbb{R}^n, \mathbb{R}_\infty^n$  are replaced by  $U, \overline{U}$ , where  $U \in \mathbb{R}^n$  is a relatively compact open set, i.e.  $\overline{U}$  is compact.

Theorem 4.1 shows that (4.1) is a rather strong condition. It should be desirable to have a characterization of the generator of a Markov semigroup relaxing (4.1), namely operators satisfying (3.4)<sup>22</sup>. In this connection the following remarks are relevant: it can be shown that a *necessary and sufficient* condition for a linear operator acting on  $C^2$ - functions and for which  $Z(1) = 0$ , is a 2nd order differential operator, is that for any  $A$  in its domain and  $x_0$  such that  $A(x_0) = 0$ , it follows that  $Z(A^3)(x_0) = 0$ <sup>23</sup>. On the other hand, (3.4) implies that for all nonpositive functions  $Z(A^3)(x_0) \leq 0$  whenever  $A(x_0) = 0$ . Therefore in theorem 4.1 the equality-sign case is characterized. To put it differently : generators of Markov semigroups that are not only differential operators, are characterized by the condition that there exist nonpositive functions  $A$  for which

$$Z(A^3)(x_0) < 0 \quad \text{when} \quad A(x_0) = 0$$

Thus the problem reduces to the characterization of such operators.

## 5. DEGENERATE ELLIPTIC EQUATIONS AND MARKOV SEMIGROUPS

In the previous section we have shown that *the generator of a Markov semigroup is a 2nd order differential operator if it is defined for  $C^2$ -functions and satisfies (4.1)*. On the other hand, as mentioned in section 1, various approaches to kinetic theory that starting from microscopic classical dynamics and imposing more or less systematic approximation schemes, lead to linear autonomous kinetic equations for particular classes of systems that are partial differential equations (see e.g. the approaches based on iteration schemes applied to the so-called generalized master equation of one or another form<sup>2-4</sup>). Therefore *they are incompatible with  $A_1 - A_4$  unless they are at most of the 2nd order with nonnegative-definite leading coefficient*.

Using the results of section 4 we shall show that under quite general conditions, *the converse is true, namely an operator of the form (4.2) generates a Markov semigroup on observables globally defined on the phase space*. Moreover conservation of positivity is essentially equivalent to the existence of an  $H$ -theorem for the adjoint semigroup. This is the subject of the next section. We consider  $\mathbb{R}^n$ , but our results are applicable to any differentiable manifold, without essential modifications, since they depend on local differentiability properties of function of  $\mathbb{R}^n$  and its local compactness.

We define

$$C^2(\mathbb{R}_\infty^n, \mathbb{C}) = \{f \in C^2(\mathbb{R}^n, \mathbb{C}) : f, \partial_i f, \partial_i \partial_j f \text{ have a finite limit at infinity}\} \quad (5.1)$$

(cf. the comments following  $A_1$  in section 2), hence  $C^2(\mathbb{R}_\infty^n, \mathbb{C})$  is identified with a subset of  $C(\mathbb{R}_\infty^n, \mathbb{C})$ ;  $C^k(\mathbb{R}_\infty^n, \mathbb{C})$  is defined similarly. These are dense subsets of  $C(\mathbb{R}_\infty^n, \mathbb{C})$ , noticing that for any  $\vec{x}_0 \in \mathbb{R}_\infty^n$ , and

$$f(\vec{x}) \equiv \begin{cases} \exp(-\|\vec{x} - \vec{x}_0\|^2) & , \vec{x} \in \mathbb{R}^n \\ 0 & , \vec{x} = \infty \end{cases} \quad (5.2)$$

$f$  is in  $C^k(\mathbb{R}_\infty^n, \mathbb{C})$  and  $f(\vec{x}_0) \neq f(\vec{x})$  if  $\vec{x}_0 \neq \vec{x}$  and using the Stone-Weierstrass theorem.

**Definition 5.1** The operator  $Z : C^2(\mathbb{R}_\infty^n, \mathbb{C}) \rightarrow C(\mathbb{R}_\infty^n, \mathbb{C})$  is defined by

$$Zf(\vec{x}) = a_{ij}(\vec{x})\partial_i\partial_j f(\vec{x}) + b_i(\vec{x})\partial_i f(\vec{x}) \quad (5.3)$$

where  $a_{ij}, b_i \in C(\mathbb{R}_\infty^n, \mathbb{C})$ . Here and in what follows the summation convention is used. By the above discussion  $Z$  is densely defined. We next prove

**Proposition 5.1**  $Z$  in (5.3) is closable.

**Proof:** (i) It is sufficient that if  $\lim_{n \rightarrow +\infty} \|f_n\| = 0$  for  $f_n \in \mathcal{D}(Z)$  and there exists  $g$  such that  $\lim_{n \rightarrow +\infty} \|Zf_n - g\| = 0$  then  $g = 0$ <sup>15</sup>. Let  $a_{ij}, b_i$  be in  $C^2(\mathbb{R}_\infty^n, \mathbb{C})$  and take  $\rho_0 \in C^2(\mathbb{R}_\infty^n, \mathbb{C})$  with

$$\rho_0(\vec{x}) > 0, \quad \lim_{\vec{x} \rightarrow \infty} \rho_0(\vec{x}) = \lim_{\vec{x} \rightarrow \infty} \partial_i \rho_0(\vec{x}) = 0, \quad \int_{\mathbb{R}^n} \rho_0(\vec{x}) d\mu(\vec{x}) = 1 \quad (5.4)$$

where  $\mu$  is the Lebesgue measure of  $\mathbb{R}^n$ . Clearly  $\rho_0$  has the form

$$\rho_0(\vec{x}) = c \exp(-\beta H(\vec{x})) \quad c, \beta \in \mathbb{R}^+ \quad (5.4')$$

and

$$\tilde{\mu} : \tilde{\mu}(E) \equiv \int_E \rho_0(\vec{x}) d\mu(\vec{x}) \quad (5.4'')$$

defines a measure on  $\mathbb{R}^n$ , extended to a regular measure on  $\mathbb{R}_\infty^n$  by putting  $p(t, \vec{x}, \infty) = 0$ . By (5.4) and Lemma 5.1 below

$$\mathcal{D}(Z), \text{ Range}(Z) \subseteq C(\mathbb{R}_\infty^n, \mathbb{C}) \subseteq L_\mu^\infty(\mathbb{R}_\infty^n) \subseteq L_\mu^2(\mathbb{R}_\infty^n) \subseteq L_\mu^1(\mathbb{R}_\infty^n) \quad (5.5)$$

each  $L_\mu^p$ -space equipped with the usual  $\|\cdot\|_p$  norm,  $p < +\infty$ .

(ii) Let  $\phi \in \mathcal{D}(Z)$  with compact support  $\Omega$ . Using (5.4) and (5.4'), integration by parts gives

$$\int \phi^* Z f_n d\tilde{\mu} = \int f_n [\partial_i \partial_j (a_{ij} \rho_0 \phi^*) - \partial_i (b_i \rho_0 \phi^*)] d\mu \equiv \int f_n Z^\dagger (\rho_0 \phi^*) d\mu \quad (5.6)$$

$$Z^\dagger (\phi \rho_0) = \rho_0 (Z\phi - 2(\beta a_{ij} \partial_j H - \partial_j a_{ij} + b_i) \partial_i \phi) + \phi Z^\dagger \rho_0 \equiv \rho_0 (Z\phi - H_i \partial_i \phi) + \phi Z^\dagger \rho_0 \quad (5.7)$$

$Z^\dagger$  being the formal adjoint of  $Z$ . Therefore, by (5.4)

$$|\int \phi^* g d\tilde{\mu}| \leq \|Zf_n - g\| \|\phi\|_1 + |\int \phi^* Z f_n d\tilde{\mu}| \xrightarrow{n \rightarrow \infty} 0$$

Thus  $\int \phi^* g d\tilde{\mu} = 0$  for  $\phi \in C_c^2(\mathbb{R}^n, \mathbb{C})$  which is dense in  $C_c(\mathbb{R}^n, \mathbb{C})$ . Therefore the result follows by the continuity of  $\|\cdot\|_2$  and Lemma 5.2 below.

(iii) For arbitrary  $a_{ij}, b_i$  in  $C(\mathbb{R}_\infty^n, \mathbb{C})$  and  $\epsilon > 0$  there exist functions  $\hat{a}_{ij}, \hat{b}_i \in C^2(\mathbb{R}_\infty^n, \mathbb{C})$  such that  $\|\hat{a}_{ij} - a_{ij}\| < \epsilon$ ,  $\|\hat{b}_i - b_i\| < \epsilon$ . Defining  $\hat{Z}$  by (5.3) in terms of  $\hat{a}_{ij}, \hat{b}_i$  we get

$$|\int \phi^* Z f_n d\tilde{\mu}| \leq \epsilon \|\phi\| (\|\partial_i \partial_j f_n\| + \|\partial_i f_n\|) + \|\phi\| \|\hat{Z} f_n\| \quad \forall \epsilon > 0$$

for any  $\phi \in C_c^2(\mathbb{R}_\infty^n, \mathbb{C})$  and we proceed as before.

Q.E.D.

**Lemma 5.1** If  $(X, \mathcal{B}, \tilde{\mu})$  is a measure space with  $\tilde{\mu}(X) = 1$  then for any  $f$  in  $L_\mu^\infty(X)$  we have  $\|f\|_p \leq \|f\|_q \quad \forall 0 < p < q \leq \infty$  hence  $(L_\mu^q(X), \|\cdot\|_q) \subseteq (L_\mu^p(X), \|\cdot\|_p)$  in a natural way<sup>14</sup>

**Lemma 5.2** If  $f \in C(\mathbb{R}^n, \mathbb{C})$ ,  $\tilde{\mu}$  is a finite measure on  $\mathbb{R}^n$  and for any  $\phi \in C_c(\mathbb{R}^n, \mathbb{C})$   $\int f(\vec{x})\phi(\vec{x})d\tilde{\mu}(\vec{x}) = 0$ , then  $f = 0$ .

Proposition 5.1 holds if  $\mathbb{R}^n, \mathbb{R}_\infty^n$  are replaced by  $U, \bar{U}$  respectively for any relatively compact open  $U \subseteq \mathbb{R}^n$ . Obviously (5.4') has to be modified. Therefore, let  $Z_{\bar{U}}$  be the restriction of  $Z$  in (5.3) on  $\bar{U}$  for any relatively compact open  $U \subseteq \mathbb{R}^n$ , and  $\tilde{Z}_{\bar{U}}$  its closure, easily seen to be the restriction of  $\tilde{Z}$  on  $\bar{U}$ . Then we have:

**Proposition 5.2** Suppose that for  $Z$  in (5.3),  $a_{ij}, b_i$  are in  $C^2(\mathbb{R}^n, \mathbb{R})$ ,  $a_{ij}$  is a nonnegative - definite matrix and  $\partial_k \partial_\ell a_{ij}$  are Hölder continuous for some positive exponent<sup>24</sup>. Then there is a (topological) base of relatively compact (open) sets  $\{U_a\}$  and a  $\lambda > 0$  such that for each  $U_a$   $\text{Range}(\lambda - \tilde{Z}_a) = C(\bar{U}_a, \mathbb{C})$ , where  $Z_a \equiv Z_{\bar{U}_a}$ .

The proof<sup>25</sup> uses the generalization of classical results concerning the solution of elliptic equations with *strictly* positive-definite 2nd order coefficient, bounded from below away from zero<sup>26</sup>, at the expense of requiring the coefficients to be  $C^2$ -functions<sup>27</sup>. Relaxing the restriction of strict positivity of  $(a_{ij})$  is important for kinetic theory, given that it is violated by important kinetic equations (e.g. the (linear) Landau equation either in phase-space or velocity space, or model equations like Kramers equation<sup>2,6,7</sup>), whereas regularity conditions are not so essential, since sufficient differentiability is often implicitly required.

In the above notation, let  $f \in C(\mathbb{R}^n, \mathbb{C})$  and  $f_a \equiv f|_{\bar{U}_a}$ . Then there exists a unique  $u_a \in \mathcal{D}(\tilde{Z}_a)$  with  $(\lambda - \tilde{Z}_a)u_a = f_a$ , hence  $\overline{\text{Range}(\lambda - Z_a)} = C(\bar{U}_a, \mathbb{C})$ . Proceeding as in the proof of theorem 3.1, condition (cii) of proposition 3.2 is *equivalent* to the nonnegative-definiteness of  $a_{ij}$  in (5.3). By Corollary 3.1,  $\tilde{Z}_a$  is the (dissipative) generator of a  $s$ -continuous contraction semigroup on  $C(\bar{U}_a, \mathbb{C})$ . Since  $(\tilde{Z}f)^* = \tilde{Z}f^*$ , and  $1 \in \mathcal{D}(Z_a)$ , by theorem 4.1  $\tilde{Z}_a$  *uniquely* defines a Markov semigroup on  $C(\bar{U}_a, \mathbb{C})$ . Restricting it on  $C(U_a, \mathbb{C})$ ,  $T_t^a$  say, we define  $(T_t f)(\vec{x}) = (T_t^a f)(\vec{x}) \quad \forall \vec{x} \in U_a$  for  $f \in C(\mathbb{R}^n, \mathbb{C})$

By the uniqueness of  $T_t^a$ ,  $T_t$  is well-defined, positivity preserving and since  $U_a$  is open,  $T_t f$  is continuous. Then for  $f \in C_c(\mathbb{R}^n, \mathbb{C})$ , its support can be covered by a finite subset of  $\{U_a\}$ ,  $U_1, \dots, U_n$  say, and  $\text{support}(T_t f) \subseteq \text{support}(f)$ , since on each  $U_a$ ,  $T_t^a$  is a Markov semigroup. Therefore

$$|T_t f(\vec{x})| \leq \max\{\|T_t^k f\|, k = 1, 2, \dots, n\} \leq \|f\|$$

hence  $T_t$  is bounded. By the remark to theorem 2.1, any  $\ell$  in  $(C_c(\mathbb{R}^n, \mathbb{C}))^*$  is biuniquely



defined by a finite measure  $\mu$ , so that

$$\ell(T_t f - f) \leq \sum_{k=1}^n \int_{U_k} d\mu(\vec{x}) |T_t^k f(\vec{x}) - f(\vec{x})| \leq \mu(\mathbb{R}^n) \sum_{k=1}^n \|T_t^k f - f\|$$

Thus  $T_t$  is  $w$ -continuous at  $t = 0$ , hence  $s$ -continuous for all  $t > 0$ . Therefore  $T_t$  is uniquely extended to  $C_0(\mathbb{R}^n, \mathbb{C})$  since  $C_c(\mathbb{R}^n, \mathbb{C})$  is dense there<sup>14</sup>, preserving the above properties (this extension is also denoted by  $T_t$ ). As in the proof of theorem A.1.1, we show that  $T_t$  satisfies (A.2.1) for some probability measure  $p(t, \vec{x}, \cdot)$  on  $\mathbb{R}^n$ , regularly extended on  $\mathbb{R}_\infty^n$  by putting  $p(t, \vec{x}, \{\infty\}) = 0$ . Thus  $T_t$  is a Markov semigroup on  $C(\mathbb{R}_\infty^n, \mathbb{C})$  with generator locally given by the closure of  $Z$  in (5.3). This completes the proof of

**Theorem 5.1**  $Z$  in (5.3) is a densely defined, closable operator on  $C(\mathbb{R}_\infty^n, \mathbb{C})$ . Its closure  $\tilde{Z}$  generates a Markov semigroup  $T_t$  on  $C(\mathbb{R}_\infty^n, \mathbb{C})$  if  $(a_{ij})$  is a nonnegative-definite matrix function,  $a_{ij}, b_i$  are in  $C^2(\mathbb{R}^n, \mathbb{R})$  and  $\partial_k \partial_\ell a_{ij}$  are Hölder continuous for some exponent in  $(0,1)$ .

*Remark:* Theorem 5.1 is valid without essential modifications on any differentiable manifold, in particular for a relatively compact open subset of  $\mathbb{R}_\infty^n$  (see the remark preceding proposition 5.2).

## 6. THE $H$ -THEOREM AND CONCLUDING REMARKS

In this section we consider arbitrary Markov semigroups on  $C(\mathbb{R}_\infty^n, \mathbb{C})$ , the generator of which *is not necessarily* a differential operator. We shall prove that *the adjoint semigroup giving the evolution of states, satisfies a general  $H$ -theorem*. Working with the adjoint semigroup, the proof turns out to be simpler and the theorem more general than that obtained directly from the kinetic equation. We introduce the measure  $\tilde{\mu}$  defined by (5.4''). Then any  $\phi \in C(\mathbb{R}_\infty^n, \mathbb{C})$  (or  $\phi \in L_\mu^1(\mathbb{R}_\infty^n)$ !) defines a bounded linear functional  $\ell_\phi$  on  $C(\mathbb{R}_\infty^n, \mathbb{C})$  via

$$\ell_\phi(A) = \int A(\vec{x}) \phi(\vec{x}) d\tilde{\mu}(\vec{x}) \quad (6.1)$$

If  $T_t$  is a Markov semigroup then by theorem A.1.1 and Fubini's theorem<sup>14,28</sup>, to  $T_t^* \ell_\phi$  corresponds uniquely the measure (cf. (A.1.4)).

$$\nu_t(E) \equiv \int p(t, \vec{y}, E) \phi(\vec{y}) d\tilde{\mu}(\vec{y}), \quad (T_t^* \ell_\phi)(A) = \int A(\vec{x}) d\nu_t(\vec{x}) \quad (6.2)$$

and we have the following

**Theorem 6.1 (H-Theorem)** Let  $T_t$  be a Markov semigroup on  $C(\mathbb{R}_\infty^n, \mathbb{C})$ , with corresponding Markov process  $p(t, \vec{x}, E)$ . If

$$p(t, \vec{x}, E) = \int_E q(t, \vec{x}, \vec{y}) d\mu(\vec{y}) \quad (6.3)$$

where  $q(t, \cdot, \cdot)$  is jointly Borel measurable, and  $\tilde{\mu}$  is an invariant measure of  $p(t, \vec{x}, E)$ , i.e.

$$\int p(t, \vec{x}, E) d\tilde{\mu}(\vec{x}) = \tilde{\mu}(E) \quad (6.4)$$

Then for any positive  $\phi \in C(\mathbb{R}_\infty^n, \mathbb{C})$ ,  $T_t^* \ell_\phi$  is defined uniquely by the density

$$\phi_t(\vec{x}) = \int q(t, \vec{y}, \vec{x}) \phi(\vec{y}) d\tilde{\mu}(\vec{y}) \quad (6.5)$$

For any convex function  $h : \mathbb{R}^+ \rightarrow \mathbb{R}$  and all nonnegative  $\phi \in C(\mathbb{R}_\infty^n, \mathbb{C})$ , with  $h \circ \phi$   $\tilde{\mu}$ -integrable,

$$H(t) \equiv \int h\left(\frac{\phi_t}{\rho_0}\right) d\tilde{\mu} \quad (6.6)$$

is a decreasing function ( $H$ -function) <sup>29</sup>.

**Proof:** (6.5) follows from (6.2), (6.3). For the second assertion we use Jensens' inequality<sup>14,30</sup>. Since  $q(t, \cdot, \vec{x})$  is  $\tilde{\mu}$ -integrable,  $E \rightarrow \int_E q(t, \vec{y}, \vec{x}) d\tilde{\mu}(y)$  defines a measure on  $\mathbb{R}^n$ , with a finite total measure which by (6.3), (6.4) is  $\int q(t, \vec{y}, \vec{x}) d\tilde{\mu}(\vec{y}) = \rho_0(\vec{x})$ <sup>31</sup>. Since  $q, \phi$  are nonnegative, Jensen's inequality and (6.5) give

$$h\left(\int \frac{q(t, \vec{y}, \vec{x}) \phi(\vec{y})}{\rho_0(\vec{x})} d\tilde{\mu}(\vec{y})\right) = h\left(\frac{\phi_t(\vec{x})}{\rho_0(\vec{x})}\right) \leq \int \frac{q(t, \vec{y}, \vec{x}) h(\phi(\vec{y}))}{\rho_0(\vec{x})} d\tilde{\mu}(\vec{y})$$

Therefore by  $\int q(t, \vec{y}, \vec{x}) d\mu(\vec{x}) = p(t, \vec{y}, \mathbb{R}_\infty^n) = 1$

$$\int h\left(\frac{\phi_t(\vec{x})}{\rho_0(\vec{x})}\right) d\tilde{\mu}(\vec{x}) \leq \int h(\phi(\vec{y})) d\tilde{\mu}(\vec{y}) = \int h\left(\frac{\phi_t(\vec{x})}{\rho_0(\vec{x})}\right) \Big|_{t=0} d\tilde{\mu}(\vec{x})$$

and since  $p(0, \vec{x}, \vec{E}) = \chi_E(\vec{x})$  by (6.3),  $q(0, \vec{x}, \vec{y}) = \delta(\vec{x} - \vec{y})$  (cf. remark (b) to theorem A.1.1). Thus  $H(t) \leq H(0)$ . If  $\phi_t \equiv S_t \phi$  then by (6.5) and (A.1.1), (6.3) implies the semigroup property for  $S_t$ , hence applying the above result to  $\phi_t$  for any  $s \geq 0$  we have

$$H(t+s) = \int h\left(\frac{S_s(S_t \phi)}{\rho_0}\right) d\tilde{\mu} \leq \int h\left(\frac{S_t \phi}{\rho_0}\right) d\tilde{\mu} = H(t)$$

Q.E.D.

*Remarks:*

(a) Equation (6.4) is equivalent to  $T_t^* \ell_1 = \ell_1$  (c.f. (6.1))

(b) When  $T_t$  is a stochastic matrix semigroup  $T_{nm}(t)$  with  $\sum_n T_{nm}(t) = 1$ , the  $H$ -theorem holds with the substitutions

$$\phi(\vec{x}) \longleftrightarrow p_n, \quad \phi_t(\vec{x}) \longleftrightarrow \sum_m T_{nm}(t) p_m \equiv p_n(t)$$

$$\rho_0(\vec{x}) \longleftrightarrow \pi_n = \sum_m T_{nm}(t) \pi_m, \quad \int (\cdot) d\tilde{\mu}(\vec{x}) \longleftrightarrow \sum_m (\cdot) \pi_m$$

The essential condition for the  $H$ -theorem is (6.4)<sup>32</sup>. To clarify its meaning we go back to diffusion-type Markov semigroups and notice that if  $a_{ij}, b_i \in \mathcal{D}(Z)$ , use of (5.4), (5.6), (5.7), (6.1) implies that under the assumptions of theorem 5.1 and for any  $f \in \mathcal{D}(Z)$

$$\ell_\phi(Zf) = \int (Z\phi - H_i \partial_i \phi) f d\tilde{\mu} + \int f \phi Z^\dagger \rho_0 d\mu \quad (6.7)$$

Suppose that  $Z^\dagger \rho_0 = 0$ . By (6.7)  $f \rightarrow \ell_\phi(Zf)$  is bounded hence it can be uniquely extended to  $C(\mathbb{R}_\infty^n, \mathbb{C})$  and therefore it belongs to  $\mathcal{D}(Z^*)$ , and

$$(Z^* \ell_\phi)(f) = \int Z^\dagger(\rho_0 \phi) f d\mu \quad \forall f \in \mathcal{D}(Z) \quad (6.8)$$

Since  $\mathcal{D}(Z)$  is dense,  $(\tilde{Z})^* = Z^*$ , hence  $\ell_\phi \in \mathcal{D}((\tilde{Z})^*)$ . Finally (6.8) can be applied to  $\phi = 1$  and therefore  $Z^\dagger \rho_0 = 0$  is equivalent to  $\tilde{\mu}$  being an invariant measure of the Markov process corresponding to  $T_t$ . But it is easily seen that  $T_t^* \ell_\phi$  is  $s$ -continuous, hence using theorem 2.1, equation (2.4), we complete the proof of

**Proposition 6.1** If  $a_{ij}, b_i$  in (5.3) are in  $\mathcal{D}(Z)$  and  $\rho_0$  in (5.4) is annuled by

$$Z^\dagger \equiv \partial_i(a_{ij} \partial_j + (\partial_j a_{ij} - b_i)) \quad (6.9)$$

$$Z^\dagger \rho_0 = 0 \quad (6.10)$$

then (i) any  $\phi \in C^2(\mathbb{R}_\infty^n, \mathbb{C})$  defines an  $\ell_\phi \in \mathcal{D}(\tilde{Z}^*)$  via (6.1) and

$$\frac{d}{dt} T_t^* \ell_\phi = (\tilde{Z})^* T_t^* \ell_\phi = Z^* T_t^* \ell_\phi \quad (6.11)$$

(ii)  $\tilde{\mu}$  in (5.4'') is an invariant measure of the corresponding Markov process.

(iii) If (6.3) holds and  $q(t, \vec{x}, \cdot)$  is a  $C^2$ -function for  $t > 0$ , then (cf.(6.5)) satisfies

$$\frac{\partial \phi_t}{\partial t} = Z^\dagger \phi_t \quad (6.12)$$

**Proof:** The first two assertions have already been proved. For (6.12), we notice that by (6.2), (6.5), (6.11),

$$\lim_{t \rightarrow t_0} \int \left( \frac{\phi_t(\vec{x}) - \phi_{t_0}(\vec{x})}{t - t_0} - Z^\dagger \phi_{t_0}(\vec{x}) \right) A(\vec{x}) d\mu(\vec{x}) = 0$$

uniformly in  $A \in C_c(\mathbb{R}^n, \mathbb{C})$ . For  $x_0 \in \mathbb{R}^n$  we take  $f \in C_c(\mathbb{R}^n, \mathbb{C})$  nonnegative, sufficiently differentiable with  $f(\vec{x}_0) > 0$  and  $A_n(\vec{x})$  a  $\delta_{x_0}$ -sequence of  $C^\infty$ -functions. If  $t_n \rightarrow t_0$  as  $n \rightarrow +\infty$ , applying the above equation to  $A_n(\vec{x})f(\vec{x})$ , written as

$$\lim_{n \rightarrow +\infty} \int f(\vec{x}) G_n(\vec{x}) A_m(\vec{x}) d\mu(\vec{x}) = 0$$

we can show from the uniform convergence with respect to  $m$  of this double sequence, that  $\lim_{n \rightarrow +\infty} G_n(\vec{x}_0) = 0$ , i.e. (6.12) holds. Q.E.D.

*Remark:* In the formalism of Refs. 6, 7  $H_i$  in (5.7) is zero (equation (2.19) of Ref.7 and the discussion following it). By (5.7), (6.9), (5.4') this *implies* (6.10). The essential content of this proposition is that *the existence of an invariant measure  $\tilde{\mu}$ , hence of an  $H$ -theorem, is supplied by the existence of an equilibrium distribution satisfying (5.4)*. Physically speaking, this may be interpreted as the stationarity of a Maxwell-Boltzmann (MB) distribution for the formal adjoint equation (6.12), if  $H$  in (5.4') is nonnegative.

At this point however it should be noticed that *although the existence of a stationary solution of (6.12) is not a strong requirement*, on the contrary, it is a physically desirable feature of classical kinetic equations, *its Lebesgue integrability* (see (5.4)), is a constraint *violated by quite simple evolution equations and for which a differential form of an  $H$ -theorem is nevertheless easily proved* (cf. (6.14) below and the discussion following it). Think for instance of the diffusion equation, even with variable coefficients, for which  $\rho_0(\vec{x}) = 1$  (see also appendix 2). Therefore, one is tempted *to relax (5.4) and keep only the stationarity of  $\rho_0$* . Then, a careful reconsideration of the proofs of theorem 6.1 and proposition 6.1 shows that *minor modifications* in their hypotheses *ensure their validity in this case as well*. This is the content of

**Corollary 6.1** With the notation of theorem 6.1 and proposition 6.1, suppose  $\rho_0$  is a nonnegative,  $C^2$ -function, bounded at infinity (or on the boundary of a relatively compact subset of  $\mathbb{R}^n$  - cf. remark to theorem 5.1) together with its first derivatives, satisfying (6.10);  $\phi$  in (6.5) has compact support;  $h(0) = 0$  for  $h$  in (6.6).

Then, (6.12) is valid and (6.4) holds *locally*, i.e.

$$\int q(t, \vec{y}, \vec{x}) \rho_0(\vec{y}) d\mu(\vec{y}) = \rho_0(\vec{x}) \tag{6.4'}$$

from which the H-theorem follows (cf.(6.6)).

We may use proposition 6.2 to get an instructive, albeit more special, differential form of the H-theorem : If  $h$  is twice differentiable, then by (6.12), at least formally

$$\frac{dH}{dt} = \int h'(\tilde{\phi}_t) Z^\dagger(\tilde{\phi}_t \rho_0) d\mu \quad (6.13)$$

where  $\tilde{\phi}_t = \phi_t/\rho_0$ ,  $h'(y) = dh/dy$ . Using (5.7), (6.10) directly and in the form  $\int h(\tilde{\phi}_t) Z^\dagger \rho_0 d\mu = 0$  we find after a straightforward but lengthy calculation,

$$\frac{dH}{dt} = - \int \rho_0(\tilde{\phi}_t) h''(\tilde{\phi}_t) a_{ij} \partial_i \tilde{\phi}_t \partial_j \tilde{\phi}_t d\mu \quad (6.14)$$

under the assumption

$$(\rho_0 a_{ij} \partial_j h(\tilde{\phi}_t) + h(\tilde{\phi}_t) H_i)|_\infty = 0 \quad (6.15)$$

(for instance if  $h$  is a  $C^1$ -function with  $h(0) = 0$ , e.g.  $h(x) = x^2$ ).

Since  $h'' \geq 0$ , *the H-theorem holds if and only if  $a_{ij}$  is a nonnegative-definite matrix* (cf. proposition 4.3 of Ref.6; for stochastic matrices see Ref.2 section V.5). This shows explicitly the close connection between *conservation of positivity* (cf. (3.4), (5.3)) and the *existence of H-functions*, though theorem 6.1 is more general. In view of the remark to proposition 6.1 and apart from regularity conditions on the coefficients of the generator  $Z$ , equation (5.3), *such an operator having a nonnegative-definite second order coefficient*, leads to a satisfactory kinetic description (c.f. end of section 2) in the sense that it *defines a Markov semigroup satisfying a general H-theorem, once the existence of a bounded at infinity equilibrium solution (possibly of the MB-type) for its formal adjoint has been assured*. As a final remark, notice that by the above discussion (cf.(6.14)), *such a solution ensures that the Markov semigroup property is equivalent to the existence of H-functions* (cf. in this respect Refs.33).

As already mentioned, *this follows if  $H_i = 0$* , equation (5.7), which is valid in the formalism developed in Refs.6, 7 thus proving that the latter provides a satisfactory kinetic description for open systems interacting with large baths at canonical equilibrium.

**Acknowledgement:** This work has been partly supported by the Euratom Fusion Programm.

## APPENDIX 1

The characterization of Markov semigroups in terms of Markov processes is well-known, but proofs are often incomplete or different because of differences in the definition of a Markov process. Here we use

**Definition A.1.1** Let  $M$  be a compact topological space, and  $B$  its Borel  $\sigma$ -algebra. Then a (time homogeneous) Markov process on  $M$  is a function  $p : \mathbb{R}^+ \times M \times B \longrightarrow \mathbb{R}$  such that

- (i)  $p(t, x, \cdot)$  is a probability measure
- (ii)  $p(t, \cdot, E)$  is a Borel function
- (iii)

$$p(t + s, x, E) = \int p(t, x, dy)p(s, y, E) \quad (\text{A.1.1})$$

For any  $f \in C(M, \mathbb{C})$

$$T_t f(x) \equiv \int p(t, x, dy)f(y) \quad (\text{A.1.2})$$

is continuous. The process is called uniformly stochastically continuous if <sup>16</sup>

$$\lim_{p \rightarrow 0^+} p(t, x, E) = 1 \quad \text{uniformly in } x \in E \quad (\text{A.1.3})$$

$T_t$  is called a Feller semigroup and we have the following theorem<sup>34,35</sup> used in the proof of theorems 3.1, 4.1

**Theorem A.1.1** Uniformly stochastically continuous Markov processes on  $M$  are in 1-1 correspondence with  $s$ -continuous Markov semigroups on  $C(M, \mathbb{C})$ , the latter being equipped with the supremum norm.

**Outline of proof:** ( $\Rightarrow$ ) It is easily shown that (A.1.2) defines a positivity and normalization preserving semigroup. By a standard argument, uniformity of the limit in (A.1.3) implies  $s$ -continuity of  $T_t$ .

( $\Leftarrow$ ) Let  $T_t$  be a Markov semigroup on  $C(M, \mathbb{C})$ . For each  $x \in M$ ,  $t \geq 0$

$$\ell : C(M, \mathbb{C}) \rightarrow \mathbb{C} : \quad \ell(f) = T_t f(x)$$

is a positive (hence bounded) linear functional on  $C(M, \mathbb{C})$ . By (2.6) and theorem 2.1 there exists a unique probability measure  $p(t, x, \cdot)$  such that (A.1.2) holds. (A.1.1) follows from the uniqueness of  $p(t, x, \cdot)$  and the semigroup property of  $T_t$ . Condition (ii) is proved by using for every compact or open  $E$ , a monotonic sequence of continuous

functions  $f_n$ , converging pointwise to  $\chi_E$ <sup>28</sup> to show that  $\lim_{n \rightarrow +\infty} T_t f_n(x) = p(t, x, E)$ , so that condition (ii) holds for such  $E$ . Then taking account of the regularity of  $p$ <sup>14</sup>, this result is extended to all Borel sets. (A.1.3) is proved by taking for every Borel set  $E$  and  $x \in E$ , an  $f \in C(M, \mathbb{R})$  vanishing outside  $E$ , and  $f(x) > 0$ , and consider the *continuous* function

$$g(y) = \begin{cases} 1, & f(y) \geq f(x) \\ \frac{f(y)}{f(x)}, & f(y) < f(x) \end{cases}$$

for which  $0 < g(y) \leq 1$  for all  $y$  such that  $f(y) > 0$ . Then it is easily shown that  $g(x) - T_t g(x) \geq 1 - p(t, x, E)$  and (A.1.3) follows by the s-continuity of  $T_t$ . Q.E.D.

*Remarks:* (a) It can be shown<sup>34</sup> that by the compactness of  $M$ , pointwise convergence in (A.1.3) is *equivalent* to uniform stochastic continuity, based on the fact that pointwise convergence of  $T_t$  for  $t = 0$  is equivalent to w-continuity for  $t = 0$ .

(b) Using (2.3) and the regularity of  $p(0, x, \cdot)$ , we get  $p(0, x, E) = \chi_E(x)$  for any Borel set  $E$ .

(c) For every (positive and/or probability) measure  $\nu$  defining uniquely  $\ell \in C^*(M, \mathbb{C})$ ,  $T_t^* \ell$  is uniquely specified by the (positive and/or probability) measure

$$\nu_t(E) = \int p(t, x, E) d\nu(x) \quad (\text{A.1.4})$$

## APPENDIX 2

Here we present one-dimensional examples of Markov semigroups, for which a *non-integrable* equilibrium solution  $\rho_0$ , satisfying (6.10) exists, but which nevertheless satisfy the requirements of corollary 6.1, hence they obey a global H-theorem (for their physical interpretation see ref.36)

$$(a) \quad ZA = (1 + x^2) \partial_x^2 A - (2\alpha - 1)x \partial_x A \quad x \in \mathbb{R}, \quad \alpha \geq -1/2$$

$$(b) \quad ZA = x^2 \partial_x^2 A + (1 - (2\alpha - 1)x) \partial_x A \quad x > 0, \quad \alpha \geq -1/2$$

The corresponding (unnormalized) equilibrium solution  $\rho_0$  of their formal adjoints are respectively

$$\rho_0 = (1 + x^2)^{-(\alpha+1/2)}, \quad \rho_0(x) = x^{-(2\alpha+1)} e^{-1/x}$$

(notice that  $H_i$  in (5.7) vanishes identically - cf. remark to proposition 6.1). It can be shown that for  $-1/2 \leq \alpha \leq 0$ , these solutions are not integrable, although they

satisfy the conditions of corollary 6.1, hence the corresponding semigroups satisfy an H-theorem in the sense of theorem 6.1. Notice that when the phase space is not  $\mathbb{R}_\infty^n$ , as in (b) above, the results of section 6 are still valid provided we replace any conditions imposed at infinity, with the same conditions on the boundary of the phase space.

## References

- <sup>1</sup> H. Risken *The Fokker-Planck equation*, Springer, Berlin (1984).
- <sup>2</sup> N.G. van Kampen, *Stochastic processes in physics and chemistry*, North Holland, Amsterdam (1992), chs.VIII, IX;
- <sup>3</sup> R. Balescu, *Equilibrium and nonequilibrium statistical mechanics*, Wiley, New York (1975).
- <sup>4</sup> The literature is extensive, see e.g. Ref.3 and P. Résibois and M. de Leener, *Classical kinetic theory of fluids*, Wiley, New York(1977); R. Kubo, M. Toda and N. Hashitsume, *Statistical Physics*, Vol II, Springer Berlin (1985).
- <sup>5</sup> C. W. Gardiner *Handbook of stochastic methods*, Springer, Berlin (1985), ch.3;
- <sup>6</sup> A.P. Grecos and C.Tzanakis, *Physica* **A151**, 61 (1988).
- <sup>7</sup> C. Tzanakis, *Physica* **A151**, 90 (1988).
- <sup>8</sup> E.B. Davies, *Comm. Math. Phys.* **39**, 91 (1974); E.B. Davies, *Math. Annalen* **219**, 147 (1976);
- <sup>9</sup> e.g N.G. van Kampen and I. Oppenheim, *Physica* **A138**, 231 (1986), section 2 and p.239 eq.(3.5); V. Rudyak and I. Ershov, *Physica* **A219**, 351 (1995), eq.(15); J. Piasecki and G. Szamel, *Physica* **A143**, 114 (1987), section 3 eq.(29); S.A. Aldeman, *J. Chem. Phys.* **64**, 124 (1976), eq.(3.19); M. Tokuyama, *Physica* **A169**, 147 (1990), eq.(4.9a).
- <sup>10</sup> A. Dimakis and C. Tzanakis, *J Physics A* **29**, 577 (1996).
- <sup>11</sup> G. Lindblad, *Comm. Math. Phys.* **48**, 119 (1976); V. Gorini, A. Kossakowski and E.C.G. Sudarshan, *J. Math. Phys.* **17**, 821 (1976); V. Gorini, A. Frigerio, M. Veri, A. Kossakowski and E.C.G. Sudarshan, *Rep. Math. Physics* **13**, 149 (1978).
- <sup>12</sup> There exists an  $A_\infty \in \mathbb{C}$ , such that for every  $\epsilon > 0$ , there exists a compact  $K \subseteq X$  with  $|A(x) - A_\infty| < \epsilon$ ,  $\forall x \in X - K$ .
- <sup>13</sup> M. Reed and B. Simon, *Methods of modern mathematical physics I: Functional Analysis*, Academic Press, New York (1974), chIV.
- <sup>14</sup> W. Rudin, *Real and Complex analysis*, McGraw-Hill, London (1970), chs. 6, 3, 2, 7.
- <sup>15</sup> K. Yosida, *Functional analysis*, Springer, Berlin (1971), chs.IX, IV, II.
- <sup>16</sup> E.B. Dynkin, *Markov Processes*, Vol I, Springer, Berlin (1965), ch.1.
- <sup>17</sup> E.B. Davies, *One-parameter semigroups*, Academic Press, London (1981), chs. 1, 2, 7.
- <sup>18</sup> R.F. Pawula, *Phys. Rev.* **162**, 186 (1967). It contains Lemma 4.1 specialized to the Kramers-Moyal expansion of the linear Boltzmann equation.
- <sup>19</sup> J.V. Pulé and A. Verbeure, *J. Math. Phys.* **20**, 2286 (1979). Lemma 4.1 is shown using a different definition of dissipativity, *a priori* stronger than (3.4).
- <sup>20</sup> E. Nelson, *Dynamical theories of Brownian motion*, Princeton University Press, Princeton (1967); its theorem 5.3 outlines a proof of theorem 4.1 here.
- <sup>21</sup> That this should follow by an explicit construction of a counter example (provided by Lemma 4.1) has been pointed to one of us (C.T.) by E.B. Davies (private communication).



<sup>22</sup>A *partial* answer is provided by the Lévy-Khinchine formula characterizing Markov semigroups generated by functions of  $\nabla \equiv (\partial_i)$ , which includes (4.2) only when  $a_{ij}$ ,  $b_i$  are constants; see e.g. M. Reed and B. Simon, *Methods of modern mathematical physics IV: Analysis of operators*, Academic Press, New York (1978), theorem XIII.53.

<sup>23</sup>M. Emery, *Stochastic calculus on manifolds*, Springer, Berlin (1989), lemma 6.1.

<sup>24</sup> $f$  is Hölder continuous with exponent  $a \in (0, 1)$  if  $|f(\vec{x}) - f(\vec{y})| \leq M\|\vec{x} - \vec{y}\|^a$  for some  $M > 0$  and  $\|\cdot\|$  is the Euclidean norm.

<sup>25</sup>L. Stoica, *Local operators and Markov processes*, Springer Lecture Notes in Mathematics vol. 816, Berlin (1980).

<sup>26</sup>R. Courant and D. Hilbert, *Methods of mathematical physics*, Vol II, Wiley, New York (1962), sections IV.2, IV.7; J.R. Mika and J. Banasiak, *Singularly perturbed evolution equations with applications to kinetic theory*, World Scientific, Singapore 1995, section 3.7.

<sup>27</sup>O.A. Oleinik and E.B. Radkevich, *Second order equations with nonnegative characteristic form*, Hogy Nauky, Moskow (1971), (in Russian), theorem 1.8.2 p.86.

<sup>28</sup>P.R. Halmos, *Measure theory*, Van Nostrand, New York (1950), sections 55, 36.

<sup>29</sup>Sometimes one defines  $H(t) = \int h(T_t A) d\tilde{\mu}$  for the observables  $A$  (see e.g. Ref.15 p.392), though this has no physical interpretation.

<sup>30</sup>If  $(X, \nu)$  is a measure space with  $\nu(X) = N$ , and  $\phi \in L^1_\nu(X)$ . Then for any real-valued convex function  $h$  defined on the range of  $\phi$ ,  $h(\int_X \phi d\nu/N) \leq \int_X h \circ \phi d\nu/N$ .

<sup>31</sup>Strictly speaking  $\int_E (\int q(t, \vec{y}, \vec{x}) \rho_0(\vec{y}) d\mu(\vec{y}) - \rho_0(\vec{x})) d\mu(\vec{x}) = 0$  for every Borel set  $E$ , so that the integrand is zero  $\mu$  - a.e. Modifying  $q(t, \vec{y}, \vec{x})$  on a set of measure zero we get the result.

<sup>32</sup>By the Banach fixed-point theorem, if (3.11) is relaxed and  $p(t, \vec{x}, \mathbb{R}^n) < 1$ , any invariant measure is unique, and if  $p(t, \vec{x}, \mathbb{R}^n) \leq a < 1$  its existence is ensured as well. However (3.11) is essential in the context of kinetic theory. Nevertheless, even in this case we do not know if this invariant measure is absolutely continuous with respect to the Lebesgue measure (cf.(5.4'')).

<sup>33</sup>P.M. Alberti and A. Uhlmann, J. Math. Phys. **22**, 2345 (1981), theorem 1.2; P.M. Alberti and A. Uhlmann, Math. Nachrichten **97**, 279 (1980), proposition 5.3.

<sup>34</sup>J. Lamberti, *Stochastic Processes*, Springer, New York (1977), sections 7.6, 7.7.

<sup>35</sup>J.A. van Casteren, *Generators of strongly continuous semigroups*, Pitnam Publishing Inc., Boston (1985).

<sup>36</sup>E. Wong, in *Proceeding of symposia in applied Mathematics* vol. XVI, AMS, Providence (1964), p.264.